

*Inventors*

Nwaonicha 10/798,796

06/01/2005

L3 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2005:813 HCAPLUS  
DOCUMENT NUMBER: 142:96313  
ENTRY DATE: Entered STN: 31 Dec 2004  
TITLE: Halogen-free ionic liquids  
INVENTOR(S): Wasserscheid, Peter; Bosmann, Andreas; Van Hal, Roy  
PATENT ASSIGNEE(S): Germany  
SOURCE: U.S. Pat. Appl. Publ., 6 pp., Cont.-in-part of Appl.  
No. PCT/EP02/10206.  
CODEN: USXXCO  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
INT. PATENT CLASSIF.:  
MAIN: C07C317-00  
SECONDARY: C23G005-00  
US PATENT CLASSIF.: 252364000  
CLASSIFICATION: 45-4. (Industrial Organic Chemicals, Leather, Fats, and  
Waxes)  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004262578	A1	20041230	US 2004-798796	20040311 <--
DE 10145747	A1	20030403	DE 2001-10145747	20010917
WO 2003022812	A1	20030320	WO 2002-EP10206	20020911

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,  
UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD,  
RU, TJ, TM  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,  
CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,  
NE, SN, TD, TG

PRIORITY APPLN. INFO.: DE 2001-10145747 A 20010917  
WO 2002-EP10206 A2 20020911

PATENT CLASSIFICATION CODES:

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2004262578	ICM	C07C317-00
	ICS	C23G005-00
	INCL	252364000
US 2004262578	NCL	252/364.000
	ECLA	C07C045/50; C07D521/00B1C3
DE 10145747	ECLA	C07C045/50; C07D521/00B1C3
WO 2003022812	ECLA	C07C045/50; C07D521/00B1C3

OTHER SOURCE(S): MARPAT 142:96313

ABSTRACT:

This invention relates to novel ionic liqs. with general formula [cation][RSO4]  
[R = branched or linear, (un)saturated, aliphatic or alicyclic functionalized or  
non-functionalized hydrocarbon chain with 3-36 C atoms] such as  
1,3-dimethylimidazoliumoctyl sulfate. These novel ionic liqs. can be used as  
solvents or solvent additives in chemical reactions, as extraction agents or as heat  
carriers.

SUPPL. TERM: halogen free imidazolium sulfate ionic liq; chem reaction  
solvent ion liq; extn agent imidazolium sulfate ionic liq

INDEX TERM: Ionic liquids  
(preparation of halogen-free ionic liqs.)

INDEX TERM: Phase transfer catalysts  
(preparation of halogen-free ionic liqs. for phase transfer  
catalysts)

INDEX TERM: Extractants  
(preparation of halogen-free ionic liqs. for solvent  
extraction  
agents)

INDEX TERM: Solvents  
(preparation of halogen-free ionic liqs. for solvents)

INDEX TERM: **445473-58-5P 502421-75-2P**  
**502421-76-3P**  
ROLE: IMF (Industrial manufacture); PREP (Preparation)  
(preparation of halogen-free ionic liqs.)

INDEX TERM: **142-31-4**, Sodium octyl sulfate **151-21-3**,  
Sodium lauryl sulfate, reactions **79917-88-7**,  
1,3-Dimethylimidazolium chloride **79917-90-1**,  
1-Butyl-3-methylimidazolium chloride  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of halogen-free ionic liqs.)

IT **445473-58-5P 502421-75-2P 502421-76-3P**  
RL: IMF (Industrial manufacture); PREP (Preparation)  
(preparation of halogen-free ionic liqs.)

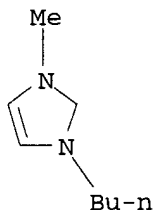
RN 445473-58-5 HCAPLUS

CN 1H-Imidazolium, 1-butyl-3-methyl-, octyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 80432-08-2

CMF C8 H15 N2



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 45102-38-3

CMF C8 H17 O4 S

Me<sup>-</sup> (CH<sub>2</sub>)<sub>7</sub>-O<sup>-</sup> SO<sub>3</sub><sup>-</sup>

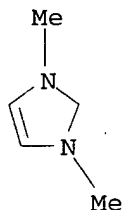
RN 502421-75-2 HCAPLUS

CN 1H-Imidazolium, 1,3-dimethyl-, octyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 45470-32-4

CMF C5 H9 N2



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 45102-38-3

CMF C8 H17 O4 S

Me- (CH<sub>2</sub>)<sub>7</sub>-O- SO<sub>3</sub><sup>-</sup>

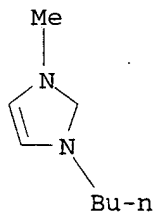
RN 502421-76-3 HCAPLUS

CN 1H-Imidazolium, 1-butyl-3-methyl-, dodecyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 80432-08-2

CMF C8 H15 N2



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 557-47-1

CMF C12 H25 O4 S

Me- (CH<sub>2</sub>)<sub>11</sub>-O- SO<sub>3</sub><sup>-</sup>

IT 142-31-4, Sodium octyl sulfate 151-21-3, Sodium lauryl sulfate, reactions 79917-88-7, 1,3-Dimethylimidazolium chloride 79917-90-1, 1-Butyl-3-methylimidazolium chloride  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of halogen-free ionic liqs.)  
RN 142-31-4 HCAPLUS  
CN Sulfuric acid, mono-octyl ester, sodium salt (8CI, 9CI) (CA INDEX NAME)

$\text{Me}^-(\text{CH}_2)_7-\text{OSO}_3\text{H}$

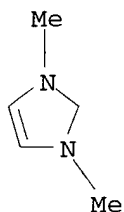
● Na

RN 151-21-3 HCAPLUS  
CN Sulfuric acid monododecyl ester sodium salt (8CI, 9CI) (CA INDEX NAME)

$\text{HO}_3\text{SO}^-(\text{CH}_2)_{11}-\text{Me}$

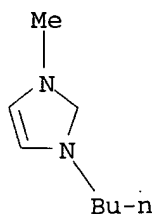
● Na

RN 79917-88-7 HCAPLUS  
CN 1H-Imidazolium, 1,3-dimethyl-, chloride (9CI) (CA INDEX NAME)



●  $\text{Cl}^-$

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE  
RN 79917-90-1 HCAPLUS  
CN 1H-Imidazolium, 1-butyl-3-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L3 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:221657 HCAPLUS

DOCUMENT NUMBER: 138:255229

ENTRY DATE: Entered STN: 21 Mar 2003

TITLE: Preparation of organic ammonium and phosphonium sulfates as ionic liquids

INVENTOR(S): Wasserscheid, Peter; Boesmann, Andreas; Van Hal, Roy

PATENT ASSIGNEE(S): Solvent Innovation GmbH, Germany

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

INT. PATENT CLASSIF.:

MAIN: C07D207-32

CLASSIFICATION: 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 22, 47, 67

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003022812	A1	20030320	WO 2002-EP10206	20020911
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
DE 10145747	A1	20030403	DE 2001-10145747	20010917
EP 1425268	A1	20040609	EP 2002-797984	20020911
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
JP 2005515168	T2	20050526	JP 2003-526888	20020911
US 2004262578	A1	20041230	US 2004-798796	20040311 <--
PRIORITY APPLN. INFO.:			DE 2001-10145747	A 20010917
			WO 2002-EP10206	W 20020911

## PATENT CLASSIFICATION CODES:

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2003022812	ICM	C07D207-32
WO 2003022812	ECLA	C07C045/50; C07D521/00B1C3
DE 10145747	ECLA	C07C045/50; C07D521/00B1C3
JP 2005515168	FTERM	4H006/AA01; 4H006/AA03; 4H006/AB40; 4H006/AB80
US 2004262578	NCL	252/364.000
	ECLA	C07C045/50; C07D521/00B1C3

&lt;--

OTHER SOURCE(S): MARPAT 138:255229

## ABSTRACT:

K+RSO4- [R = (unsatd.) aliphatic or alicyclic, (functionalized) hydrocarbon chain having between 3-36 C atoms; K = quaternary ammonium, phosphonium, imidazolium, pyridinium, pyrazolium, triazolium], were prepared Thus, 1,3-dimethylimidazolium chloride in CH<sub>2</sub>Cl<sub>2</sub> was treated portionwise with Na octylsulfate followed by stirring for 40 h to give 80% 1,3-dimethylimidazolium octylsulfate. The novel ionic liqs. can be used as solvents or solvent additives in chemical reactions, as extracting agents or as heat transfer media.

SUPPL. TERM: org ammonium phosphonium sulfate prepn ionic liq;  
imidazolium alkylsulfate prepn ionic liq;  
butylmethylimidazolium octylsulfate prepn ionic liq; solvent  
additive extg agent heat transfer medium imidazolium  
alkylsulfate

INDEX TERM: Transition metals, uses  
ROLE: CAT (Catalyst use); USES (Uses)  
(catalysts, solvents; preparation of organic ammonium and  
phosphonium sulfates as ionic liqs.)

INDEX TERM: Polymerization  
(oligomerization, solvents; preparation of organic ammonium  
and  
phosphonium sulfates as ionic liqs.)

INDEX TERM: Extractants  
Heat transfer agents  
Ionic liquids  
Phase transfer catalysts  
Solvents  
(preparation of organic ammonium and phosphonium sulfates as  
ionic liqs.)

INDEX TERM: Amide group  
Esterification  
Hydroformylation  
Isomerization  
(solvents; preparation of organic ammonium and phosphonium  
sulfates as ionic liqs.)

INDEX TERM: **445473-58-5P 502421-75-2P**  
**502421-76-3P**  
ROLE: CAT (Catalyst use); RGT (Reagent); SPN (Synthetic  
preparation); TEM (Technical or engineered material use);  
PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of organic ammonium and phosphonium sulfates as  
ionic liqs.)

INDEX TERM: **142-31-4, Sodium octylsulfate 151-21-3,**  
Sodium laurylsulfate, reactions **79917-88-7,**  
1,3-Dimethylimidazolium chloride **79917-90-1,**  
1-Butyl-3-methylimidazolium chloride  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of organic ammonium and phosphonium sulfates as

ionic liqs.)

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S): (1) Abramzon, A; ZH PRIKL KHIM (LENINGRAD) 1999, V72(4), P666 HCAPLUS  
 (2) Acep Inc & Cnrs; WO 9940025 A 1999 HCAPLUS  
 (3) Anon; PATENT ABSTRACTS OF JAPAN 1993, V017(594)  
 (4) Bolle, B; MEM SERVICES CHIM 1953, V38, P159  
 (5) Bonilha, J; J PHYS CHEM 1989, V93(1), P367 HCAPLUS  
 (6) Corkill; TRANS FARADAY SOC 1966, V62, P987 HCAPLUS  
 (7) Cuccovia, I; J CHEM SOC PERKIN TRANS 2 2000, 9, P1896 HCAPLUS  
 (8) Guilloteau-Bertin, B; EUR J ORG CHEM 2000, 8, P1391 HCAPLUS  
 (9) Jokela, P; J PHYS CHEM 1987, V91(12), P3291 HCAPLUS  
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 (11) Kloubek, J; CS 111918 A 1964 HCAPLUS  
 (12) Meguro, K; NIPPON KAGAKU ZASSHI 1959, V80, P818 HCAPLUS  
 (13) Nippon Oil Co Ltd; GB 1440238 A 1976 HCAPLUS  
 (14) Olivier, H; US 6245918 B1 2001 HCAPLUS  
 (15) Packter, A; J PHARM PHARMACOL 1963, V15, P317 HCAPLUS  
 (16) Proctr & Gamble Ltd; GB 1050791 A 1966 HCAPLUS  
 (17) Solvent Innovation Gmbh; EP 1182196 A 2002 HCAPLUS  
 (18) Solvent Innovent Gmbh; EP 1182197 A 2002 HCAPLUS  
 (19) Tomasic, V; BER BUNSEN-GES PHYS CHEM 1997, V101(12), P1942 HCAPLUS  
 (20) Yu, Z; J PHYS CHEM 1990, V94(9), P3675 HCAPLUS

IT 445473-58-5P 502421-75-2P 502421-76-3P  
 RL: CAT (Catalyst use); RGT (Reagent); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of organic ammonium and phosphonium sulfates as ionic liqs.)

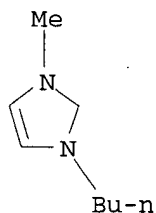
RN 445473-58-5 HCAPLUS

CN 1H-Imidazolium, 1-butyl-3-methyl-, octyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 80432-08-2

CMF C8 H15 N2



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 45102-38-3

CMF C8 H17 O4 S

Me- (CH<sub>2</sub>)<sub>7</sub>-O- SO<sub>3</sub><sup>-</sup>

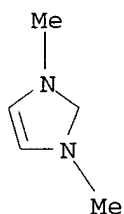
RN 502421-75-2 HCAPLUS

CN 1H-Imidazolium, 1,3-dimethyl-, octyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 45470-32-4

CMF C5 H9 N2



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 45102-38-3

CMF C8 H17 O4 S

Me- (CH<sub>2</sub>)<sub>7</sub>-O- SO<sub>3</sub><sup>-</sup>

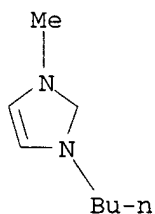
RN 502421-76-3 HCAPLUS

CN 1H-Imidazolium, 1-butyl-3-methyl-, dodecyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 80432-08-2

CMF C8 H15 N2



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

CRN 557-47-1



CMF C12 H25 O4 S

 $\text{Me}-(\text{CH}_2)_{11}-\text{O}-\text{SO}_3^-$ 

IT 142-31-4, Sodium octylsulfate 151-21-3, Sodium laurylsulfate, reactions 79917-88-7, 1,3-Dimethylimidazolium chloride 79917-90-1, 1-Butyl-3-methylimidazolium chloride  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of organic ammonium and phosphonium sulfates as ionic liqs.)  
 RN 142-31-4 HCAPLUS  
 CN Sulfuric acid, monooctyl ester, sodium salt (8CI, 9CI) (CA INDEX NAME)

 $\text{Me}-(\text{CH}_2)_7-\text{OSO}_3\text{H}$ 

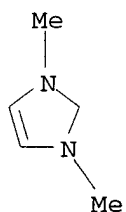
● Na

RN 151-21-3 HCAPLUS  
 CN Sulfuric acid monododecyl ester sodium salt (8CI, 9CI) (CA INDEX NAME)

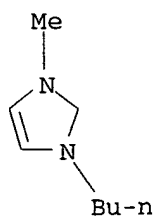
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● Na

RN 79917-88-7 HCAPLUS  
 CN 1H-Imidazolium, 1,3-dimethyl-, chloride (9CI) (CA INDEX NAME)

● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE  
 RN 79917-90-1 HCAPLUS  
 CN 1H-Imidazolium, 1-butyl-3-methyl-, chloride (9CI) (CA INDEX NAME)



● Cl<sup>-</sup>

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE